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["Toward the Systematic Generation of Hypothetical Atomic Structures: Geometric Motifs and Neural Networks."](#)

Abstract: Materials discovery, a multidisciplinary process, now increasingly relies on computational methods. We can now rapidly screen materials for desirable properties by searching materials databases and performing high-throughput first-principles calculations. However, high-throughput computational materials discovery pipelines are bottlenecked by our ability to hypothesize new structures, as these approaches to materials discovery often presuppose that a material already exists and is awaiting identification. In contrast to this assumption, synthesis efforts regularly yield materials that differ substantially from the structures in databases of previously known materials. In this talk, we discuss strategies for generating hypothetical atomic structures using the concepts of geometric motifs (the recurring patterns of atoms in materials) and neural networks that can manipulate discrete geometry (tensor field networks).